DOE CONDENSED MATTER SCIENCE REVIEW

Condensed Matter Theory

Description: There are three major areas of research within the Condensed Matter Theory group:

1. Theory of strongly correlated electron systems aimed at understanding the transport, excitation spectra, and correlation functions of low-dimensional metals and magnetic materials.
2. Statistical mechanics of complex systems, including networks, and the application of methods of theoretical physics to selected problems in molecular biology and economics.
3. First-principles electronic structure theory directed towards understanding the electronic and magnetic properties of surfaces, nanostructures, and bulk systems, and the interpretation of experimental data.

Program Highlights:

- Non-perturbative methods based on the Bethe ansatz and the Random Phase Approximation are being used to study the optical conductivity, dynamical magnetic susceptibility, and single-electron spectral function of various strongly correlated quasi-one-dimensional magnets and Mott insulators [*PRL,PRB* (submitted)].
- Developed a theory for the electron smectic fixed point of the stripe phases of doped layered Mott insulators, which exhibited a stable anisotropic non-Fermi liquid phase in the presence of a spin gap, and more conventional Fermi-liquid behavior otherwise [*PRL 85, 2160 (2000)*].
- Exactly solved models of market price fluctuations [*Physica A 278, 571 (2000)*] and a stochastically-directed sandpile related to self-organized criticality [*PRE 63, 26111 (2001)*]. Introduced the concept of a " knowledge network" [Phys. Rev. Lett. (accepted)]. A characteristic correlation pattern was discovered in several biochemical networks operating in living cells and shown to affect their specificity and stability [*Science (accepted)*].
- Used a combination of first-principles and model calculations to study materials in external fields [*Chem. Phys. Lett. 315, 167 (1999*], the mechanical stability of phases [*PRB 64, 144107 (2001)*], and dynamical effects such as self-trapping of excitons [*PRB 62, 12589 (2000)*].
- Major invited review article on *Transition-Metals and Their Alloys* published in *Solid State Physics* **56** (2001) summarizing the current understanding, and based in large part on work done at BNL.

Impact:

- The concepts of stripe phases and "bad" metals introduced earlier continue to stimulate experimental and theoretical work. The experimental evidence in favor of this unconventional behavior continues to grow.
- First-principles calculations predicted the existence of new phases and helped elucidate the properties of MgB_2 observed by various experimental probes.
- Predictions based on the non-perturbative approaches have been successfully tested experimentally.

Interactions:

- Close ties to various experimental groups, both at BNL and elsewhere.
- Collaborations with theory groups throughout the world.
- More than 35 active collaborators (see next page).

Personnel (current):

A. M. Tsvelik (group leader), M. Blume (on leave), V. J. Emery, S. S. Maslov, R. E. Watson, M. Weinert (on leave); Post-docs: J. Bhassen, B. Narozhny, V. Perebeinos, G. Schneider, R. Werner; Student: S. Carr.

Recognition:

- Emery awarded the 2001 Buckley Prize and elected to the American Academy of Arts and Sciences.
- 71 invited talks and colloquia/seminars in last 3 years.

Budget: $1077K

Condensed Matter Theory

Scientific Staff

A. M. Tsvelik (Group Leader)	Strongly correlated electron systems, low-dimensional magnetism, disordered systems, field theory.
M. Blume (on leave)	Theory of x-ray and neutron scattering.
V. J. Emery	Strongly correlated electron systems, low-dimensional magnetism, statistical mechanics.
S. S. Maslov	Theory of complex systems, interdisciplinary applications, statistical mechanics.
R. E. Watson	First-principles electronic structure theory of alloys.
M. Weinert (on leave 9/01)	First-principles electronic structure theory of surfaces, alloys, and nanostructures.

Post Docs:

Guenter Schneider	First-principles electronic structure theory of complex materials.
Ralph Werner	Strongly correlated electron systems and magnetism.
Vasili Perebeinos (arrived 4/01)	First-principle electronic structure theory.
Boris Narozhny (arrived 10/01)	Strongly correlated low-dimensional electron systems.
Joe Bhassen (arrived 11/01)	Strongly correlated low-dimensional electron systems.

Other funding:

- LDRD funding for transport and disorder in low-dimensional systems, and for electronic properties of nanostructures. ($200K)

Future Directions:

- Significantly strengthen our efforts in the physics of low-dimensional models with the addition of F. Essler to the Group (01/02).
- Extend work on the statistical mechanics of networks and the applications to biological systems to soft condensed matter.
- Play a major role in the nanoscience effort at BNL by collaborating with and providing theoretical guidance to the experimental efforts in Physics, Materials Science, NSLS, and the new Materials Center.
- Initiate a strong visitors' program to bring together theorists (and experimentalists) working in low-dimensional correlated systems for extended periods. A proposal for an Institute of Strongly Correlated and Complex Systems has been submitted (October, 01)
- Search for a new hire in theory of electronic structure.

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Collaborators:
P. B Allen, SUNY at Stony Brook, USA.
M. Alatalo, Helsinki Institute of Physics, Finland.
L. H. Bennett, NIST, USA.
G. Bihlmayer, Forschungszentrum Juelich, Germany.
S. Bluegel, University of Osnabrueck, Germany.
J.-S. Caux, University of Oxford, UK.
S.-W. Chan, Columbia University, USA.
P. Coleman, Rutgers University, USA.
F. H. L. Essler, University of Warwick, UK.
J. Fajer, Chemistry Department, BNL, USA.
H. Fehske, University of Bayreuth, Germany.
G. Fernando, University of Connecticut, USA.
T. Giamarchi, Ecolé Normalé Superieur, (Paris, France).
A. O. Gogolin, Imperial College (London, UK).
M. Holicki, University of Bayreuth, Germany.
H. J. F. Jansen, Oregon State University, USA.
P. M. Johnson, SUNY Stony Brook, USA.
S. Ketteman, IMPKIKS, Dresden (Germany).
A. Klümper, University of Dortmund, Germany.
I. I. Kogan, University of Oxford, UK.
V. Kravtsov, ICTP (Trieste, Italy).
K. K. Likharev, SUNY at Stony Brook, USA.
A. Mayr, SUNY Stony Brook, USA.
A. A. Nersesyan, ICTP (Trieste, Italy).
M. Newton, Chemistry Department, BNL, USA.
M. Pederson, Naval Research Laboratory, USA.
C. Pépin, Saclay (France).
R. Podloucky, University of Vienna, Austria.
J. Redinger, Technical University Vienna, Austria.
K. Sneppen, Nordita, Copenhagen, Denmark.
C. Tang, NEC Research Institute, Princeton, NJ, USA.
N. Taniguchi, University of Hiroshima (Japan).
D. A. Tennant, University of Oxford, UK.
K. Uchinokura, University of Tokyo, Japan.
Y.-C. Zhang, University of Fribourg, Switzerland.
A. Zheludev, ORNL, TN, USA.

Examples of internal BNL collaborations:

- *Stripe correlations in $La_{2-x}Sr_xNiO_4$:* Emery and Tsvelik collaborate with Neutron (Tranquada), X-ray (Hill), and Powder Diffraction (Vogt) Groups.
- *Superconductivity in MgB_2:* Schneider, Weinert, and Perebeinos collaborate with Powder Diffraction (Vogt), Electron Spectroscopy (Johnson, Strongin, Valla), and Electron Diffraction (Zhu) Groups.
- *Conductivity of ultrathin films:* Maslov collaborates with Electron Spectroscopy Group (Strongin, Homes) and NSLS (Carr).
- *Giant dielectric response in $CaCu_3Ti_4O_{12}$:* Werner and Schneider collaborate with Neutron (Electron Spectroscopy) and Powder Diffraction (Vogt) Groups.
- *Superconductivity and Properties of Sr_2RuO_4:* Werner collaborates with X-ray Group (Hill).
- *Photohole lifetime in Gd:* Weinert collaborates with Electron Spectroscopy Group (Johnson, Valla).
- *Haldane gaps in nickelates:* Maslov collaborates with Neutron Scattering Group (Zheludev, Zaliznyak).
- *Electronic and Magnetic Properties of Nanostructures:* Weinert, Watson, and Schneider collaborate with X-ray Scattering (Hill), NSLS (Kao, Vescovo), and Electron Diffraction (Zhu) Groups.
- *Properties of $La(Ni,Sn)_{5+x}$:* alloys: Schneider collaborates with Powder Diffraction Group (Vogt).

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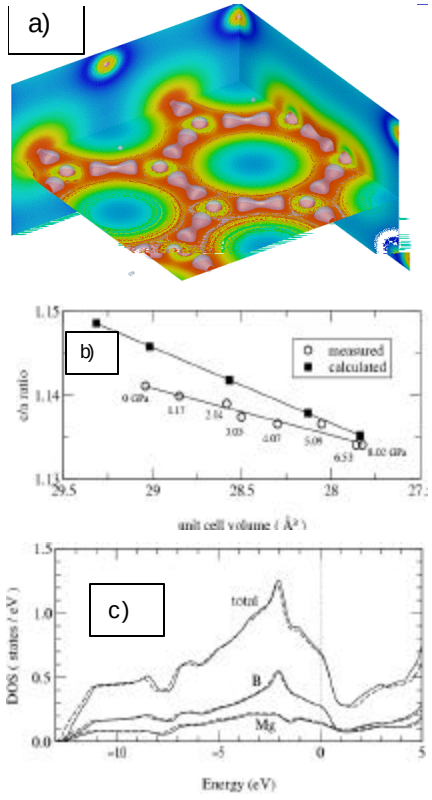
Program Highlights:

Charge Inhomogeneity

In the past few years very strong experimental evidence has been found for static or dynamic charge inhomogeneity in several strongly correlated electronic systems, particularly in high-temperature superconductors, manganites, and quantum Hall systems. The charge degrees of freedom of a doped Mott insulator are confined to an array of self-organized structures. In two-dimensions, these structures are linear and are known as stripes. Quite generally, the quantum mechanical ground states, and the thermodynamic phases which emerge from them, can, on the basis of broken symmetries, be characterized as electronic liquid crystal states. A theory was developed for the electron smectic fixed point of the stripe phases of doped layered Mott insulators that demonstrated that in the presence of a spin gap, three phases generally arise: (a) a smectic superconductor, (b) an insulating stripe crystal, and (c) a smectic metal. The latter phase is a stable two-dimensional anisotropic non-Fermi liquid. In the absence of a spin gap there is also a more conventional Fermi-liquid-like phase. The smectic superconductor and smectic metal phases (or glassy versions thereof) may have already been seen in Nd-doped $La_{2-x}Sr_xCuO_4$.[Emery, et al., *Phys. Rev. Lett. 85, 2160 (2000)*]

Superconducting, Electronic and, Structural Properties of MgB_2



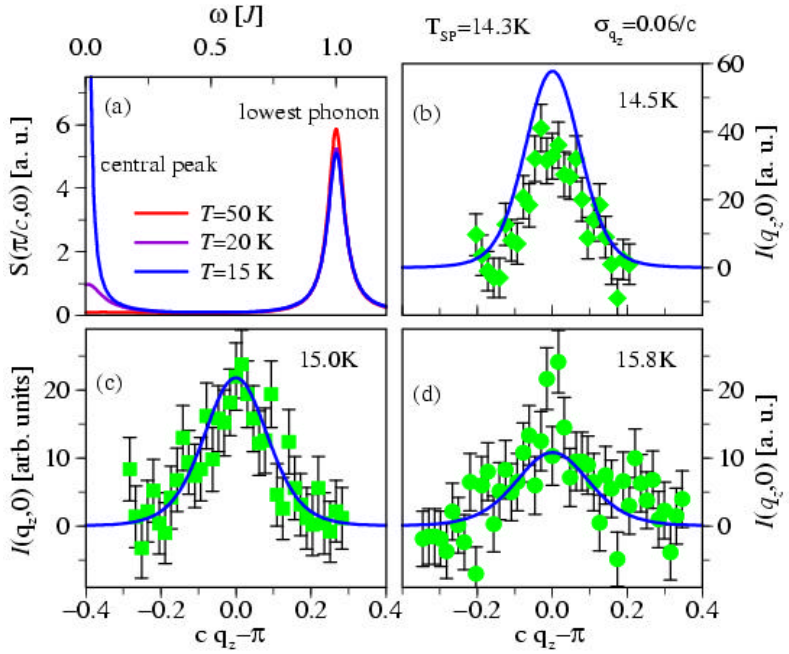
The recent discovery of superconductivity in MgB_2 has received a tremendous amount of attention. Research at BNL was characterized by the close collaboration between experiment and theory (Schneider) and contributed significantly to our current understanding of this exciting new superconducting material. First-principles electronic structure calculations based on Density Functional Theory and the Generalized Gradient Approximation were shown to give an excellent description of the electronic and structural properties of MgB_2. One crucial question regarding the nature of superconductivity concerns the character of the electronic states near the Fermi level and theory identified these states to be mostly Boron p_{xy}. The calculated valence charge density of MgB_2 is shown in panel a, with the B p_{xy} states (in the Boron plane) emphasized as iso-surfaces.

Using high resolution x-ray emission and absorption, and by comparison to calculation, the states at the Fermi level were indeed identified as being of B p_{xy} origin [McGuinness, et al., *Europhysics Letters 56, 112 (2001)*]. In another collaboration between experiment and theory, polarized electron energy loss spectroscopy at the B K-edge and calculations was used to identify the orbital symmetry of B p hole states [Zhu, et al., *Phys. Rev. Lett*. (submitted)].

Calculated bulk modulus and lattice parameters as a function of pressure were found to be in excellent agreement with experiment (panel b). Together with the pressure dependence of the density of states (DOS) shown in panel c, DOS at 0 Gpa (full lines) and 8 GPa (dashed lines), we were able to show that the pressure dependence of the superconducting properties of MgB_2 is consistent with BCS theory [Vogt, et. al, *PRB 63, 220505(R) (2001)*].

Spin-Phonon Coupling in a Spin-Peierls System

The random phase approximation (RPA) has been shown to be applicable to the spin-phonon coupling in the spin-Peierls system $CuGeO_3$. The correlations of the quasi one-dimensional magnetic sub-system are described exactly for the *XY* model and for Heisenberg chains via a complete diagonalization of finite systems. The resulting temperature and frequency-dependent line shapes of dimer-dimer correlation functions are used as input in the RPA equations. The results for $CuGeO_3$ clarify the general physics of so called central peak structural phase transitions, as driven by correlation-induced electro- or magneto-elastic excitations. The hardening of phonons and the critical excitations as a consequence of a coupling-induced magneto-elastic mode must be consistently described.



The results are summarized in the adjacent figure. Panel (a) shows the RPA dynamic lattice structure factor with parameters relevant for $CuGeO_3$. The temperature effects on the lowest Peierls active phonon mode are only of the order of <5%. Significant quasi-elastic weight appears as the temperature approaches T_{SP}=14.4 K, resulting from new magnetoelastic excitations. Panels (b)-(d) show constant energy scans of the quasi-elastic peak from theory [blue lines, Holicki, Fehske, and Werner, *PRB 63, 174417 (2001)*] and from neutron scattering [green symbols, Braden, et al., *Phys. Rev. Lett., 80, 3634 (1998)*] at different temperatures. The curves are convoluted with the experimental resolution. The fit in (d) fixes the amplitude, while the curves in (b) and (c) are parameter free. The discrepancy in panel (b) stems from critical fluctuations since the critical region has been determined to be $T_{SP} \pm 0.4$ K.

Quasi-1D Materials

The general theory describing ordered phases of quasi-1D materials based on combination of Bethe ansatz technique with Random Phase Approximation (RPA) was suggested to explain characteristic features of quasi-1D materials in their ordered state. Phase transitions in quasi-1D materials differ from phase transitions in isotropic systems in that in the former case the transition develops as an instability of a highly collective 1D state. As a result, the ordered state exhibits a peculiar blend of one- and three-dimensional features. Among other things, the theory predicts special excitation branches that exist only in quasi-1D S=1/2 antiferromagnets and systems with spin-Peierls ordering. These excitations correspond to longitudinal fluctuations of the order parameter; they have been experimentally observed in $CuGeO_3$ and $BaCu_2Si_2O_7$ [Zheludev, A., et al., *Phys. Rev. Lett. 81, 5410 (1999), Phys. Rev. B 59, 11432 (1999)*]. The theoretical predictions were also tested for the *S*=1 magnetic material Nd_2BaNiO_5 (the Haldane chain) [Zheludev, A., et al., *Phys. Rev. B 61, 11601 (2000)*]. The theoretical predictions for the spectral functions for charge density wave insulators obtained by the form factor method gave a good agreement with ARPES data for $PrBa_2Cu_3O_7$ [Essler, Tsvelik, *Phys. Rev. Lett, Phys. Rev. B,* (submitted)] and the Bechgaard salts.

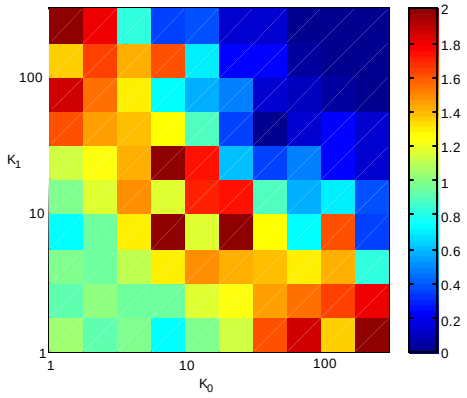
Statistical physics of networks

Extracting hidden information from knowledge networks:

We introduced a concept of *knowledge networks* [S. Maslov and Y-C. Zhang, *accepted for publication in Phys. Rev. Lett (2001)*]. The information contained in connectivity pattern of such a network allows one to reconstruct individual properties of its nodes. The technique for such reconstruction introduced in our work is of potential relevance for biological networks (e.g. that of physical interactions in a large set of biomolecules) , and the internet commerce. In this last case it allows one to predict individual tastes of customers based on a sparsely connected network of their opinions on products, services, or each other. Two distinct phase transitions occur as the density of edges in this network is increased: above the first one – the macroscopic prediction of node characteristics becomes possible, while above the second - all missing information can be uniquely reconstructed. We illustrated our ideas using a simple Gaussian model, which was studied using both field-theoretical methods and numerical simulations.

Specificity and stability in topology of protein networks:

Molecular networks guide the life of a living cell on multiple levels: its metabolic and signaling pathways are shaped by the network of interacting proteins [T. Ito, *et al , Proc. Natl. Acad. Sci. USA, **98**, 4569 (2000)*], whose production, in their turn, is controlled by the genetic regulatory network. To address topological properties of these two networks we quantified the correlations between connectivities of their interacting nodes [S. Maslov and K. Sneppen, *UC Santa Barabara, ITP preprimt NSF-ITP-01-78 (2001)*]. In the figure we plot the ratio $P(K_0,K_1)/P_{uncorr}(K_0,K_1)$, where $P(K_0,K_1)$ is the probability that a pair of proteins with connectivities K_0 and K_1 interact with each other in the real network, while $P_{uncorr}(K_0,K_1)$ is the same probability in the absence of correlations.



We found that for both studied networks links between highly connected proteins are systematically suppressed. In the figure this suppression is visualized as a large blue (standing for ratio less than one) area in the upper right corner of the figure. On the other hand the likelihood of connections between nodes of intermediate connectivities is systematically enhanced as evidenced by a red area in the middle of the figure.This type of correlation pattern reduces the number of short loops and clustering in the network, and thus decreases the likelihood of biologically undesirable cross talk, while enhancing the overall specificity and stability of the cell.

Publications:

FY1999

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